Sensitivity Analysis in Air Quality Modeling
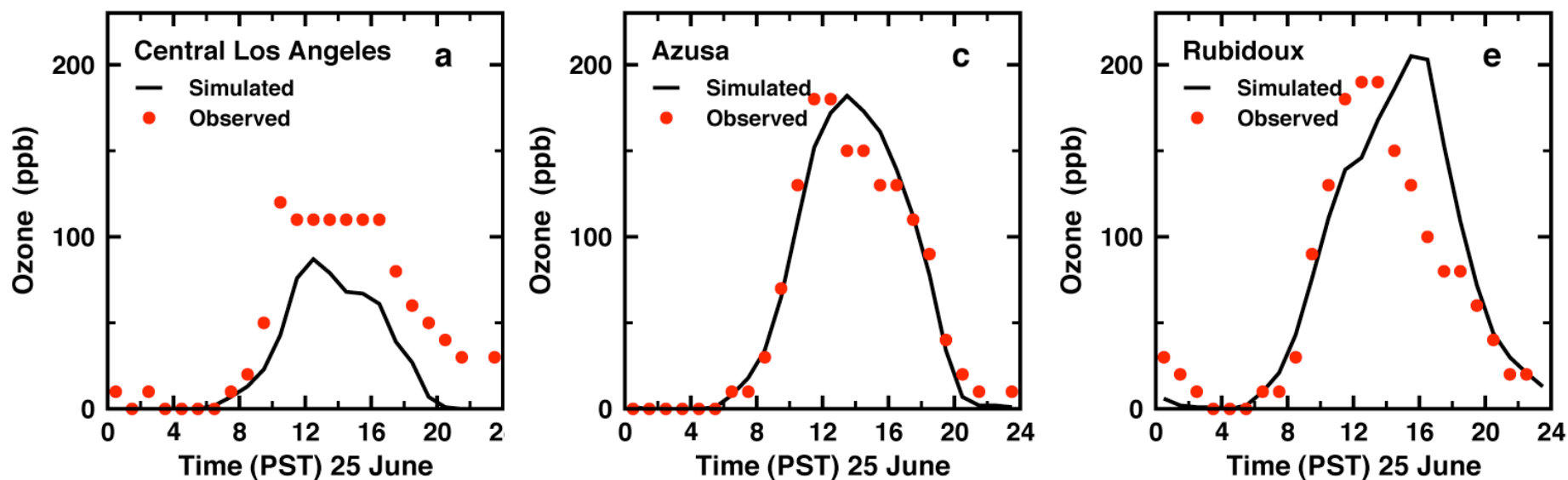

Prof. Robert Harley

University of California, Berkeley

harley@ce.berkeley.edu

Air Quality Models

- Analyze & synthesize understanding of
  - Emissions
  - Atmospheric chemistry
  - Meteorology
  - Deposition
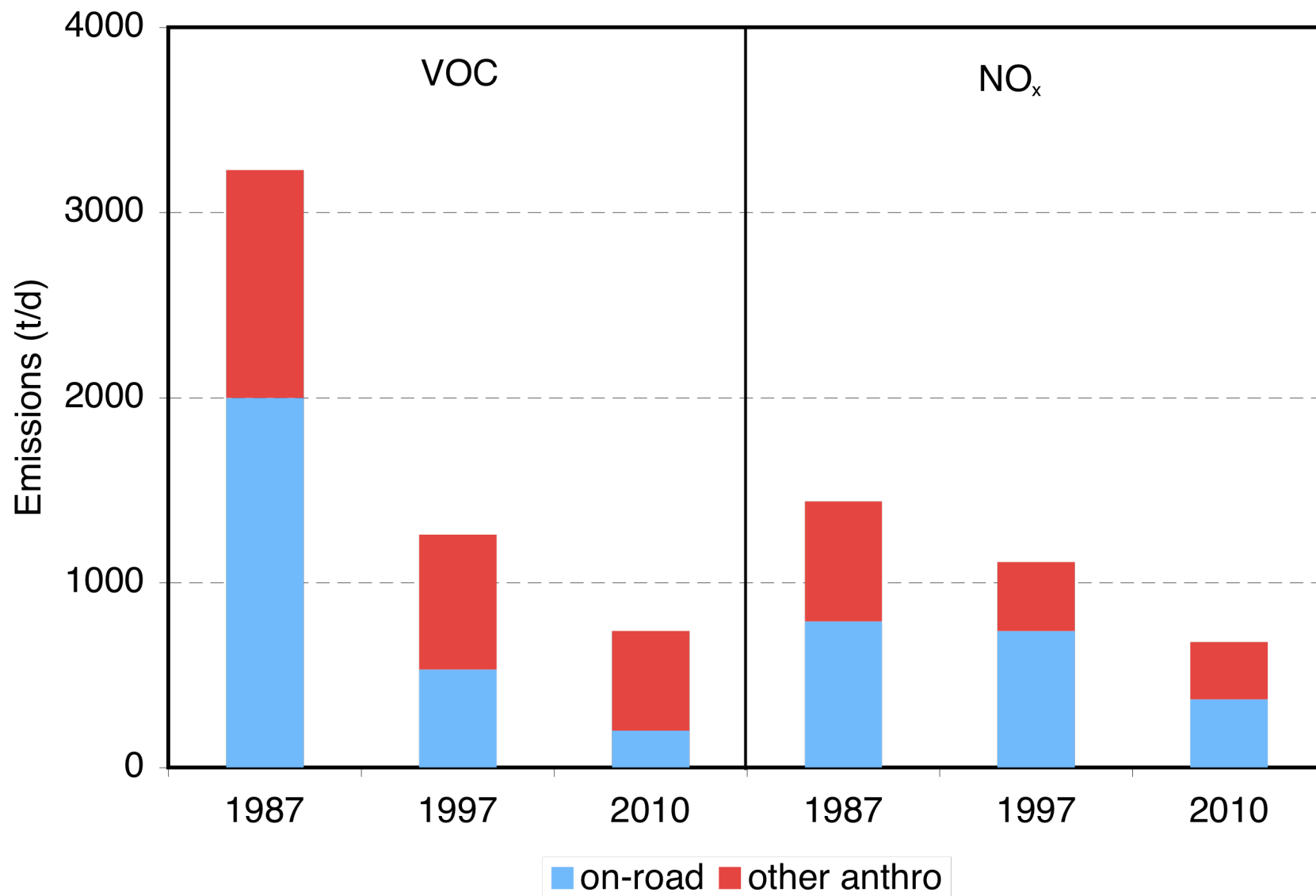- Demonstrate future attainment of air quality standards

Observed and Predicted O$_3$

Historical 1987 O$_3$ episode (Martien et al. *ES&T* 2003)
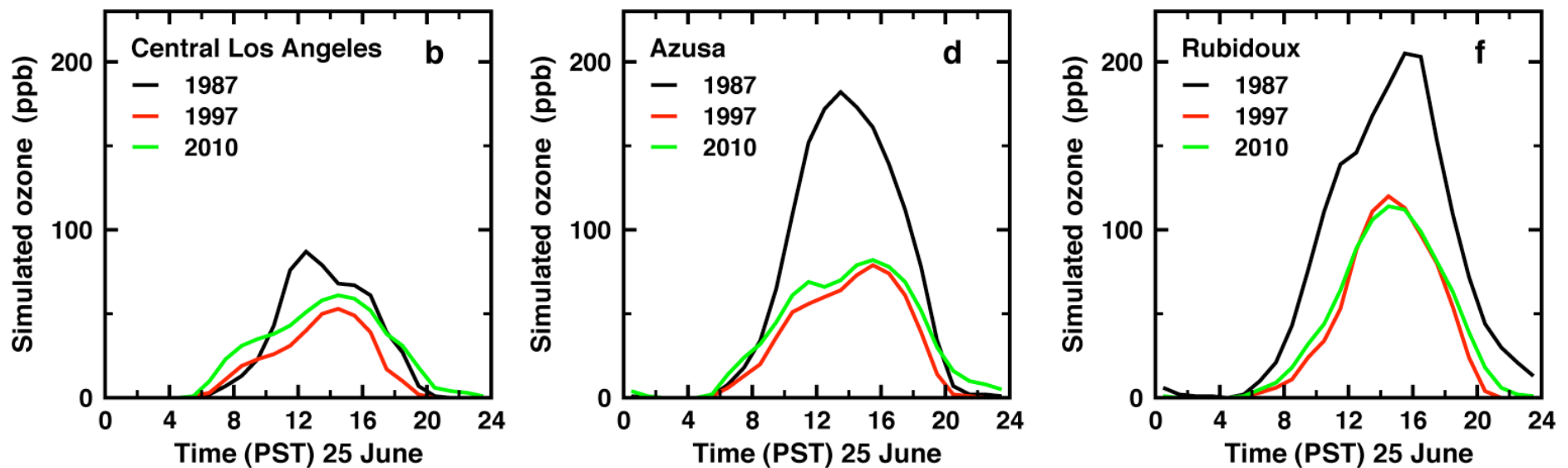Model performance (37 sites, O$_3$ > 60 ppb):
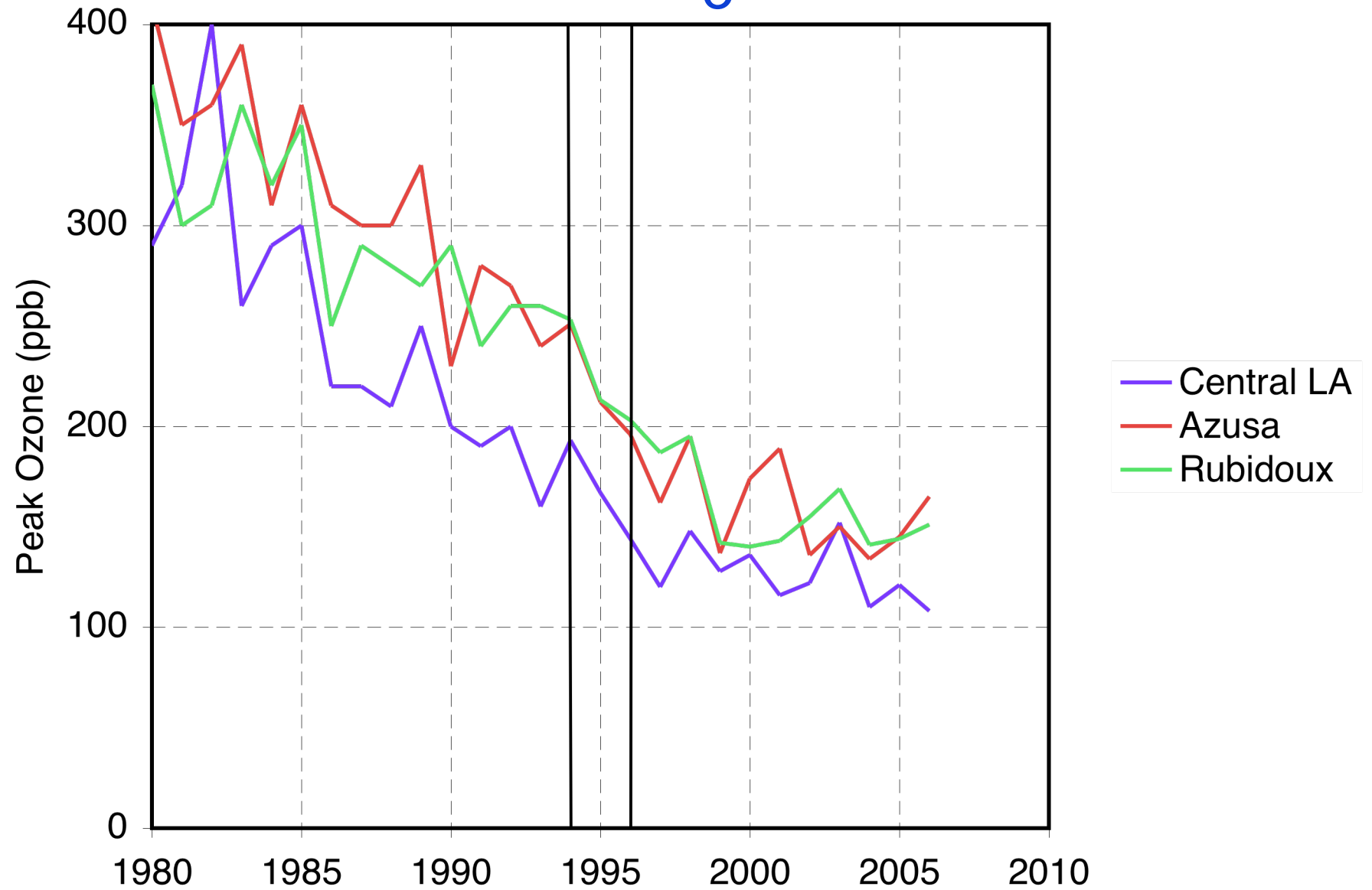Bias = +6%; Gross error = 41%

Emission Scenarios

Sources: Harley et al. (*ES&T* 1997) for 1987; 2003 AQMP for 1997 & 2010

Predicted O$_3$ Response to Emission Changes

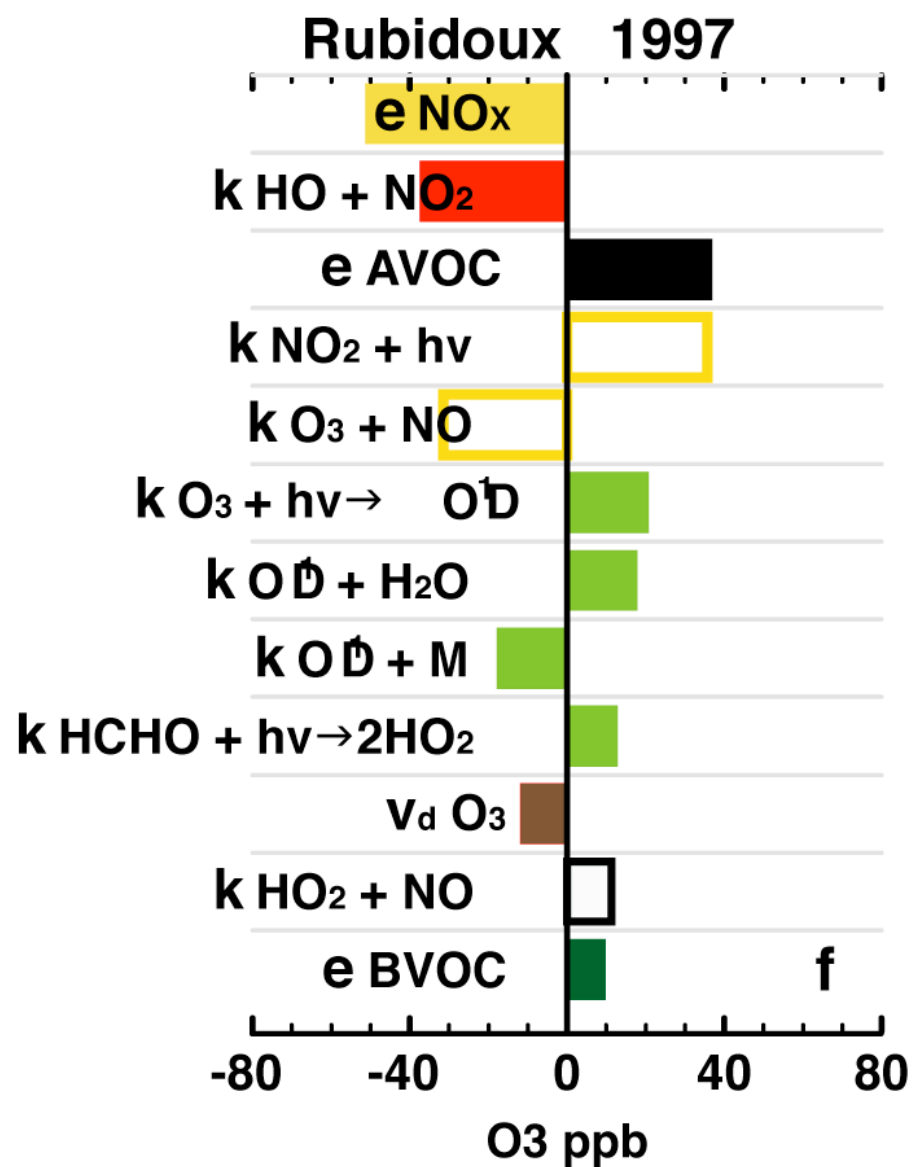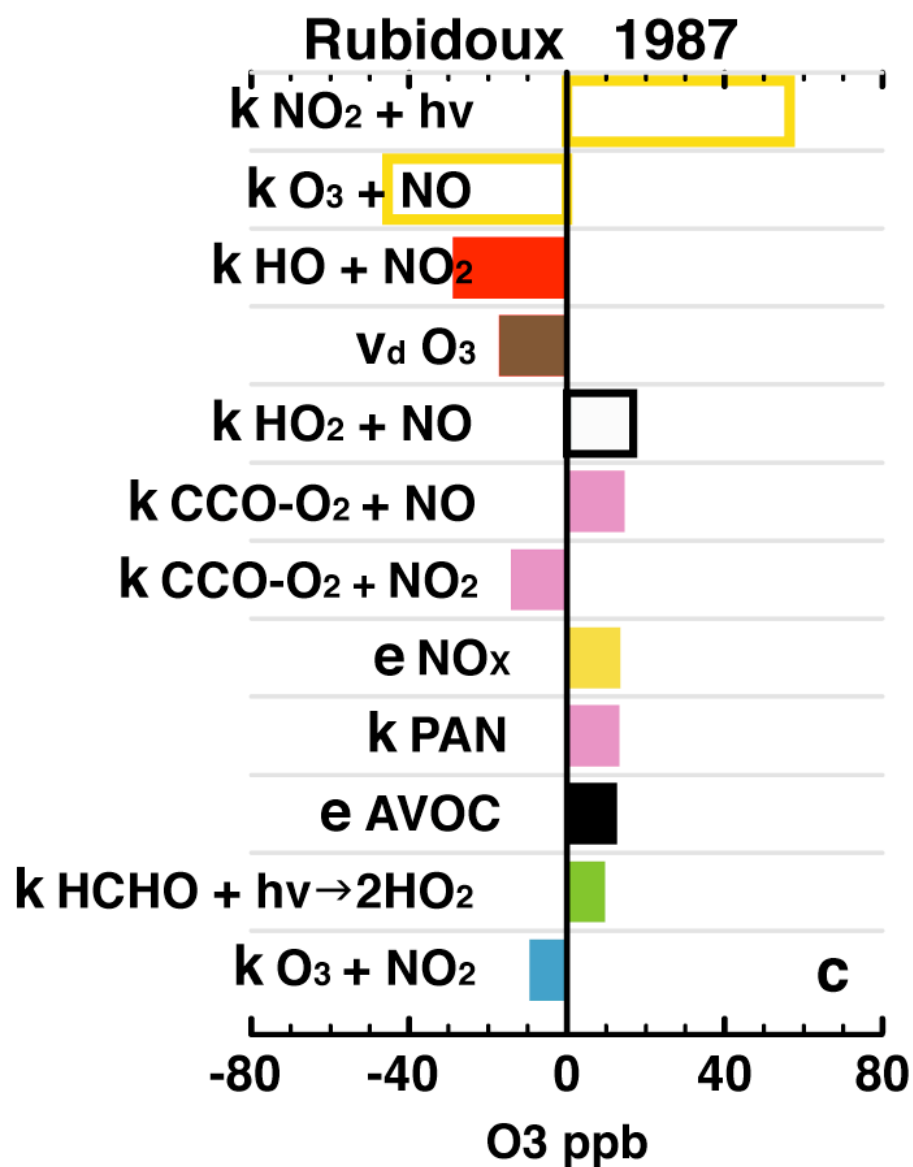Martien and Harley (*ES&T* 2006)

Observed O₃ Trends

Sensitivity Analysis

- What is model response to input data?
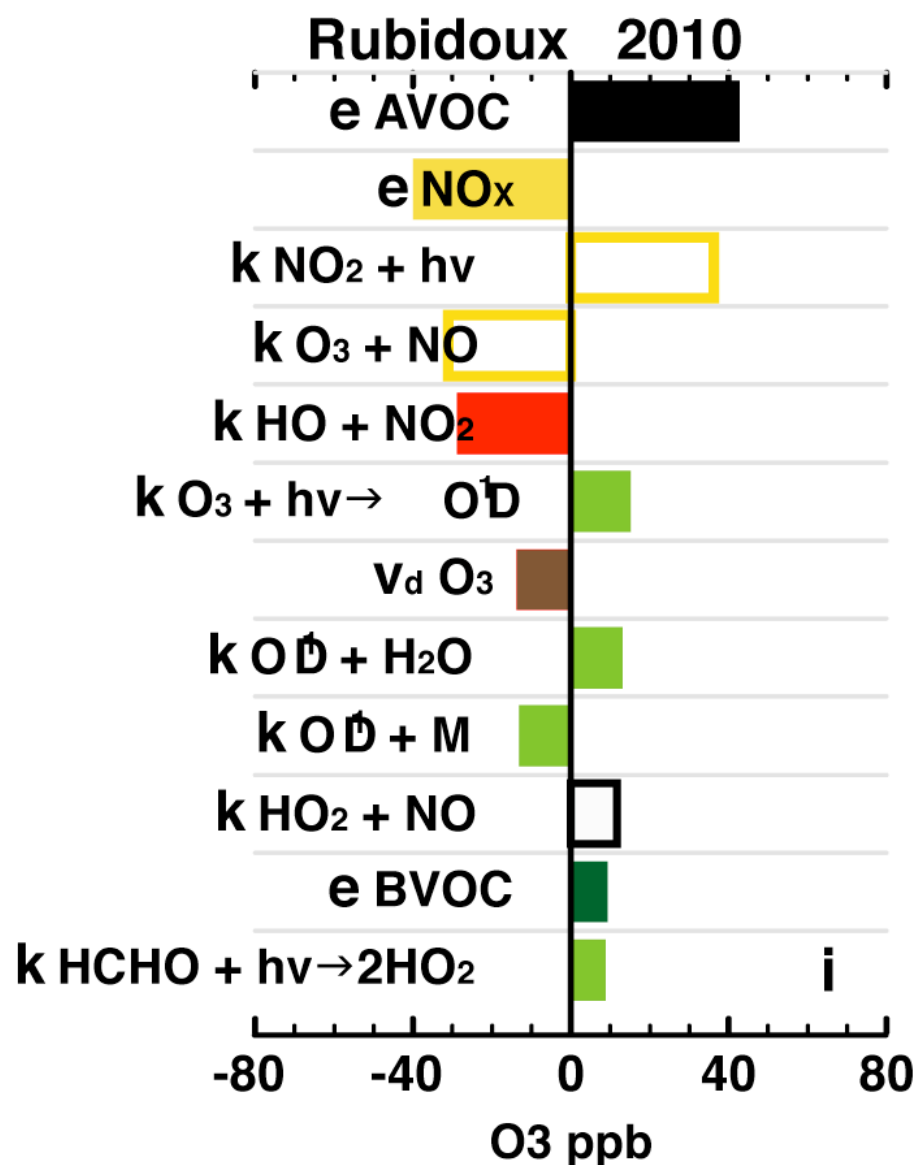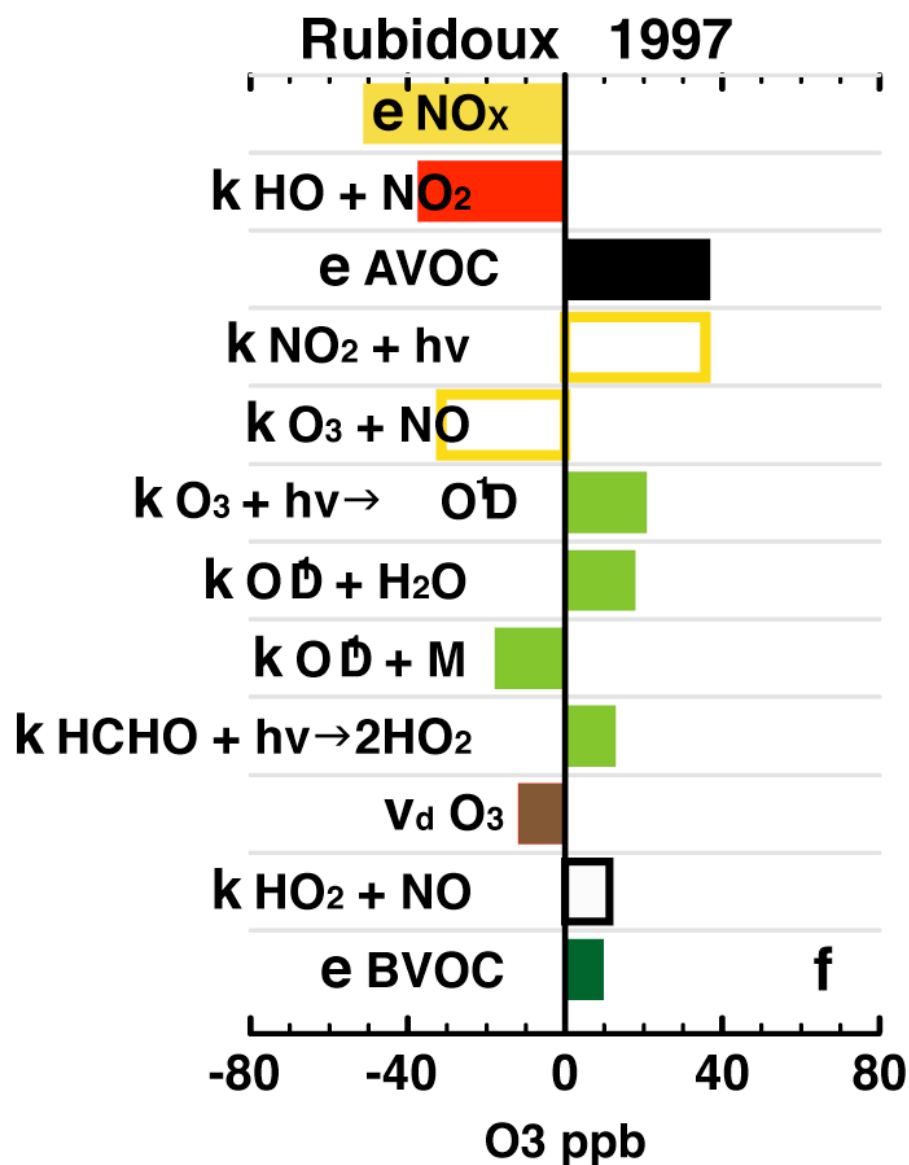
$$s_{ij} = \frac{\partial C_i}{\partial \lambda_j}$$

- Used adjoint method to calculate s_{ij} for 900 model inputs (BC, IC, E, k, v_d)

- Three emission scenarios (1987, 1997, 2010)

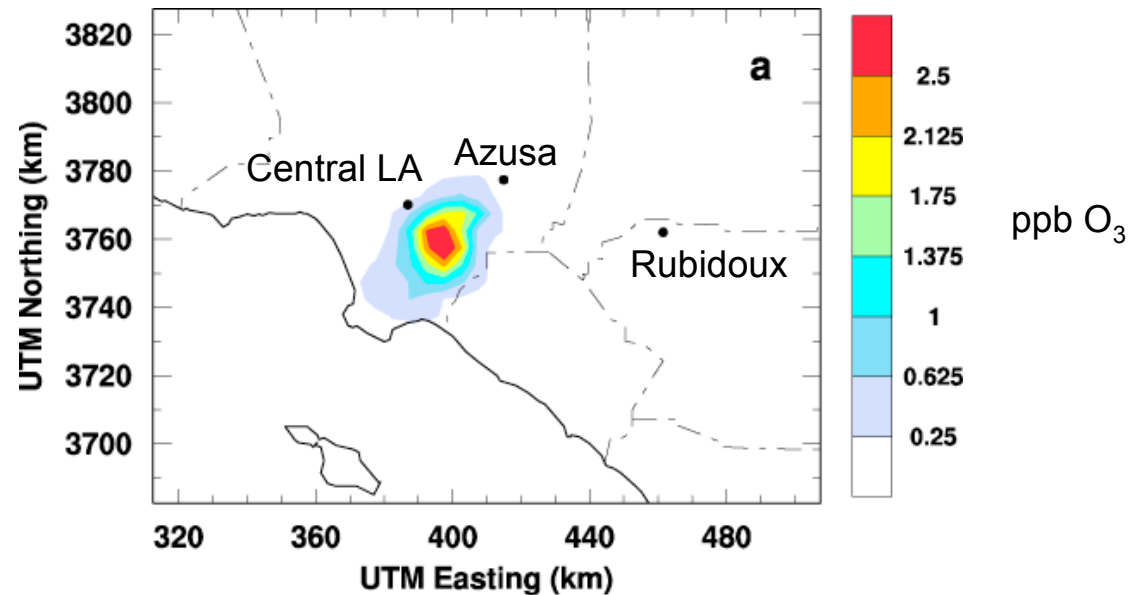- See Martien and Harley (*ES&T* 2006)

O₃ Sensitivity (Ranked)

Rubidoux   1987

k NO₂ + hv	
k O₃ + NO	
k HO + NO₂	
vd O₃	
k HO₂ + NO	
k CCO-O₂ + NO	
k CCO-O₂ + NO₂	
e NOx	
k PAN	
e AVOC	
k HCHO + hv→2HO₂	
k O₃ + NO₂	c

O3 ppb

Rubidoux   1997

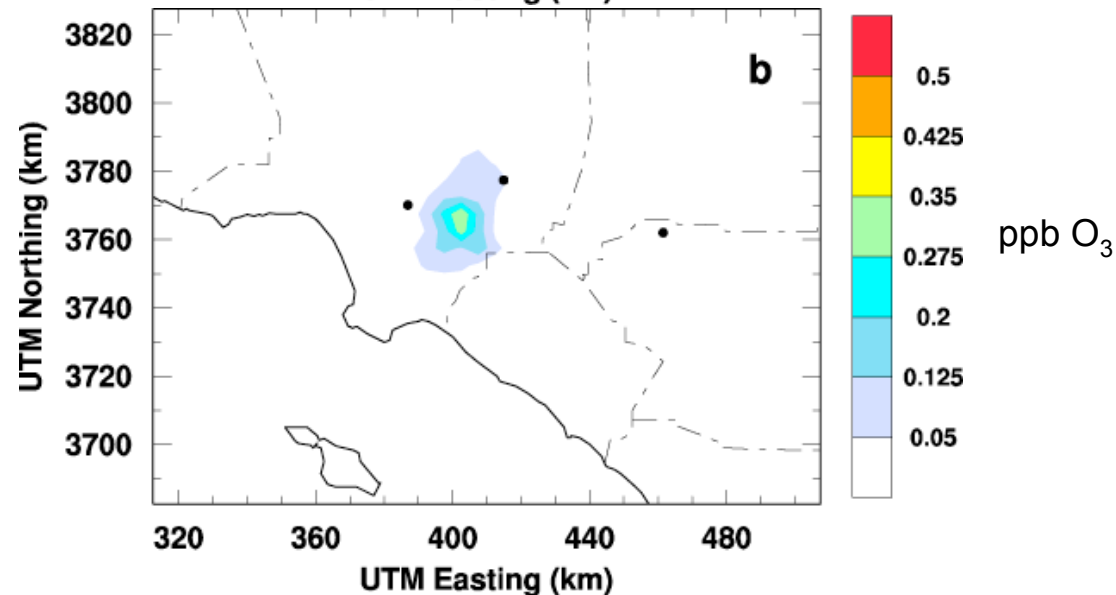|	
e NOx	
k HO + NO₂	
e AVOC	
k NO₂ + hv	
k O₃ + NO	
k O₃ + hv→ O¹D	
k O¹D + H₂O	
k O¹D + M	
k HCHO + hv→2HO₂	
vd O₃	
k HO₂ + NO	
e BVOC	f

O3 ppb

O$_3$ Sensitivity (Ranked)

Contributions to $\partial O_3 / \partial E_{VOC}$

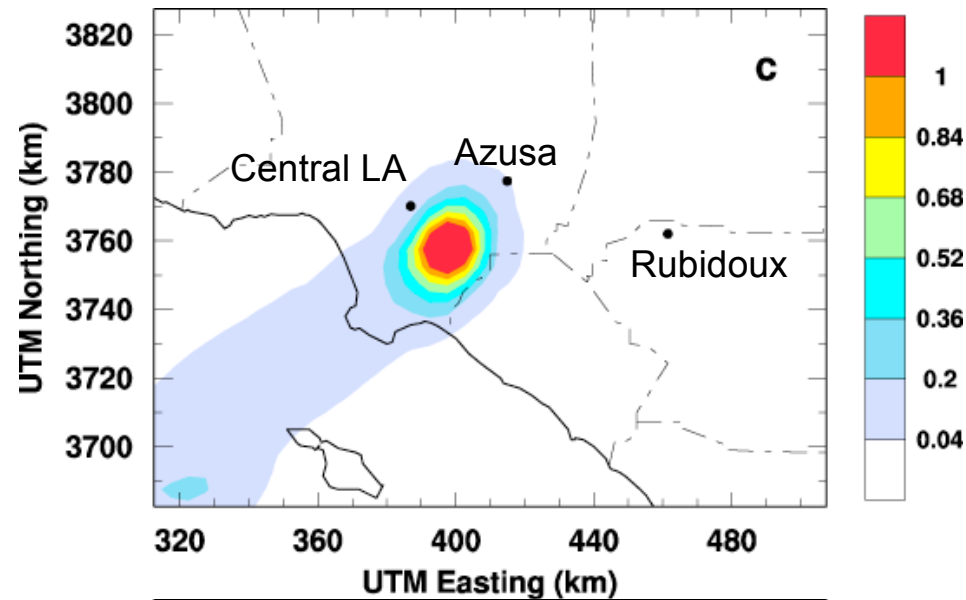Anthropogenic
(AVOC)

Biogenic
(BVOC)
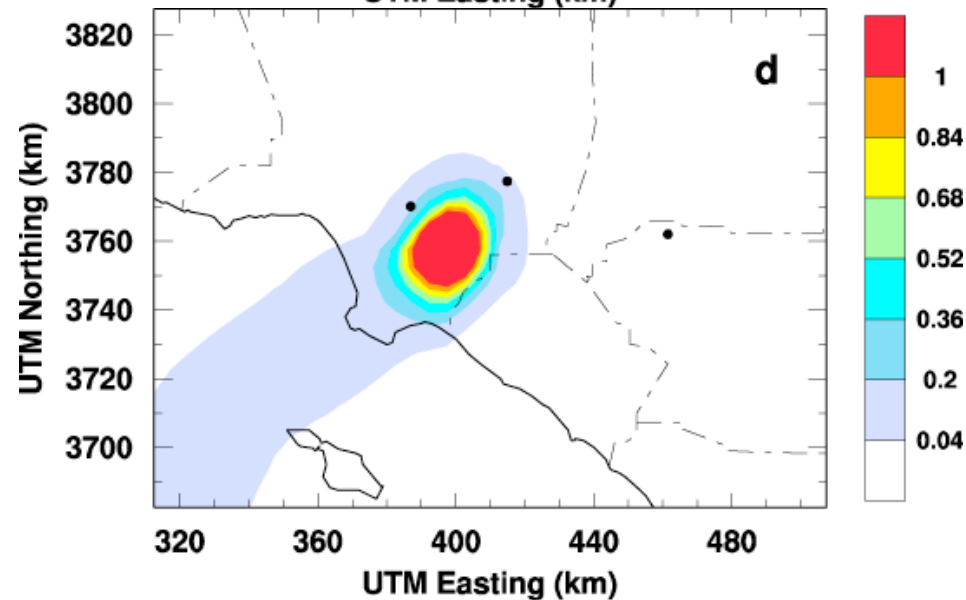
Potential Sensitivity

- Previous results show effects of <u>multiplicative</u> scaling of parameters λ_j

- Can also calculate potential sensitivity to <u>additive</u> perturbations to λ_j

- Example: effect of adding emissions where $E = 0$ in base case?
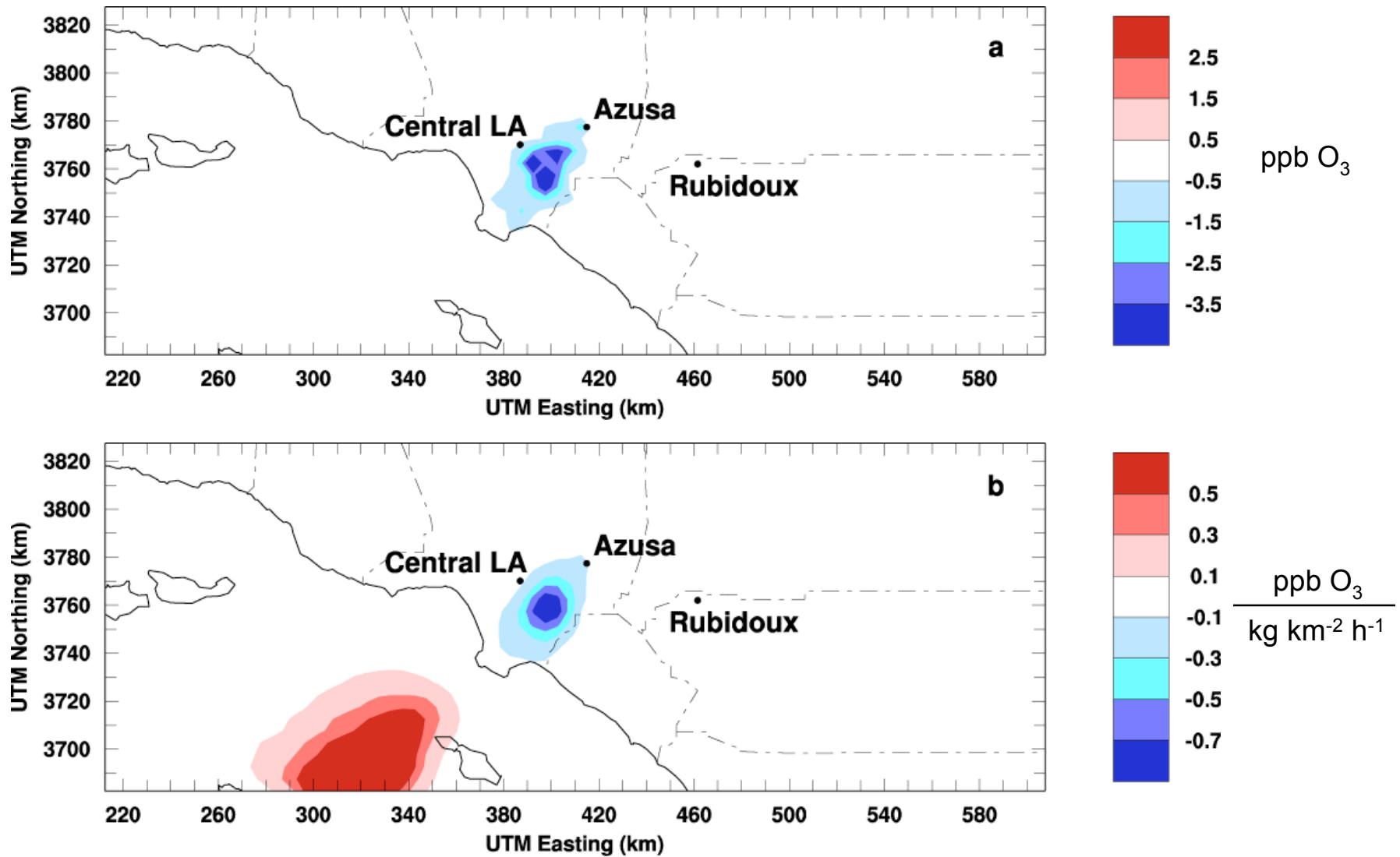
Potential Sensitivity to E$_{VOC}$

Propene

Isoprene
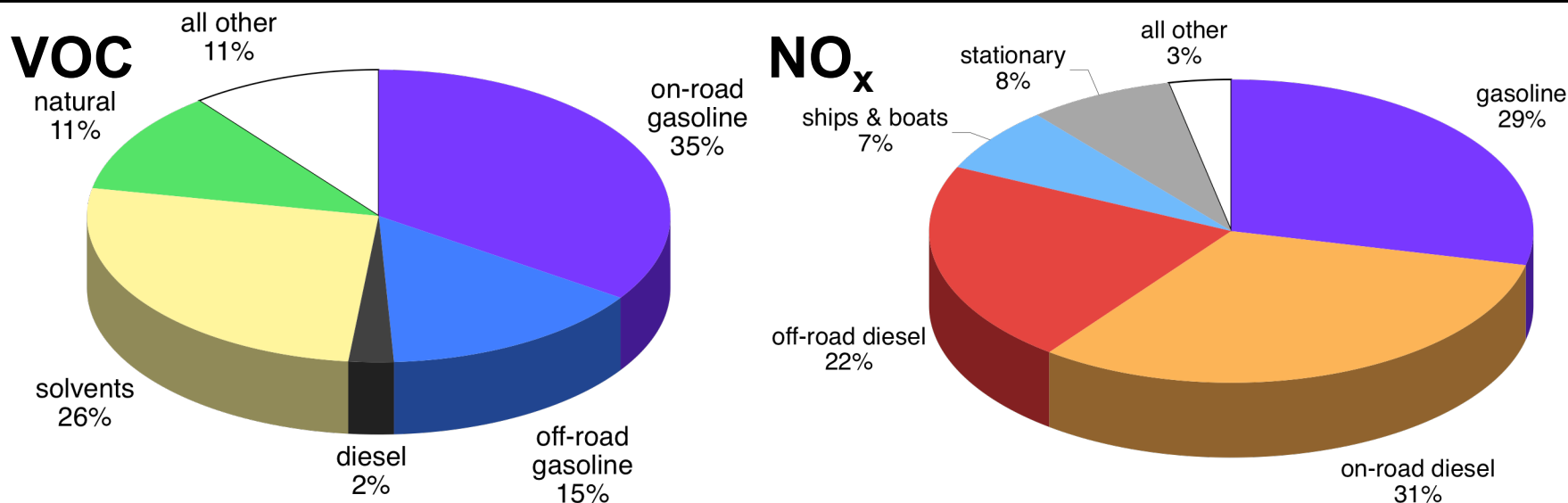
$$\frac{\text{ppb O}_3}{\text{kg km}^{-2}\text{ h}^{-1}}$$

Actual vs Potential Sens to E_{NOx}

Summary

- Adjoint method used to study O_3 sensitivity to many model inputs

- Anthropogenic emissions found to be highly influential (also uncertain!)

- Mapped source regions that affect air quality at specified locations

Emission Inventory (2005)

VOC
- all other 11%
- natural 11%
- solvents 26%
- diesel 2%
- off-road gasoline 15%
- on-road gasoline 35%

NO$_x$
- stationary 8%
- ships & boats 7%
- all other 3%
- gasoline 29%
- off-road diesel 22%
- on-road diesel 31%

- Annual average emissions for South Coast Air Basin

- VOC = 770 ton/day; mainly gasoline and solvents

- NO$_x$ = 960 ton/day; mainly diesel and gasoline combustion

- Source: CARB (2006) Air Quality Almanac